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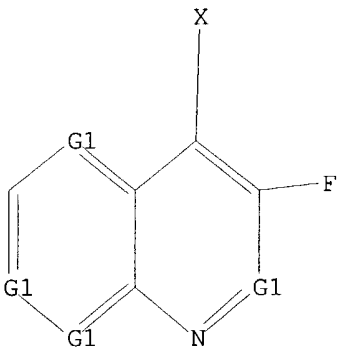


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G1 C,N


Structure attributes must be viewed using STN Express query preparation.


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=> file ca


=> s l3
L4           40 L3

=> s l3/prep
             40 L3
        3150725 PREP/RL
L5           22 L3/PREP
                   (L3 (L) PREP/RL)

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L5 ANSWER 1 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 137:247717 CA
TITLE: Preparation of 4-piperazinoquinolines which inhibit phosphorylation of a PDGF receptor
INVENTOR(S): Scarborough, Robert M.; Pandey, Anjali
PATENT ASSIGNEE(S): Millennium Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 151 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

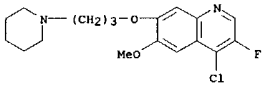
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072578	A2	20020919	WO 2002-US7187	20020308
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003004158	A1	20030102	US 2002-94191	20020308

PRIORITY APPLN. INFO.: US 2001-273951P P 20010308
OTHER SOURCE(S): MARPAT 137:247717
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; V = O, S, N(CN); W = (un)substituted 1,4-piperazinediyl, 1,4-homopiperazinediyl; X = H, TZ, F, Cl; Z = OH, CN, CHO; T = c1-16 alkylidene optionally interrupted by O, S, CO2, OCO, CO; R1 = H, (un)substituted C1-16 alkyl, C2-16 alkenyl, etc.; R2 = H, (un)substituted C1-16 alkyl, C2-16 alkenyl, etc.; R3-R6 = H, halo, alkyl, etc.] which inhibit phosphorylation of a PDGF receptor to hinder abnormal cell growth and cell wandering, and a method for preventing or treating cell-proliferative diseases such as arteriosclerosis, vascular reobstruction, cancer and glomerulosclerosis, were prepd. Thus, reacting 4-chloro-6-methoxy-7-(3-piperidylpropoxy)quinoline-3-carbonitrile (prepn. given) with N-(4-isopropoxyphenyl)piperazinecarboxamide hydrochloride in the presence of K2CO3 in DMF afforded 69% II which showed IC50 of 0.134 .mu.M and 0.060 .mu.M in MG63 w/human plasma phosphorylation assay and in HR5 phosphorylation assay, resp.
IT **460088-42-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of 4-piperazinoquinolines which inhibit phosphorylation of a PDGF receptor)
RN 460088-42-0 CA

L5 ANSWER 1 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
CN Quinoline, 4-chloro-3-fluoro-6-methoxy-7-[3-(1-piperidinyl)propoxy]- (9CI)
(CA INDEX NAME)

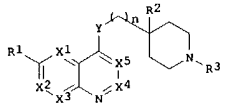


L5 ANSWER 2 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 136:386033 CA
TITLE: Heterocyclylalkyl piperidine derivatives, particularly 4-[3-(quinolin-4-yl)propyl]piperidine-4-carboxylic acids, their preparation and compositions containing same, for use as antibacterials.
INVENTOR(S): Bacque, Eric; Carry, Jean-Christophe; El-Ahmad, Youssef; Evers, Michel; Hubert, Philippe; Malleron, Jean-Luc; Mignani, Serge; Pantel, Guy; Tabart, Michel; Viviani, Fabrice
PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
SOURCE: PCT Int. Appl., 362 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040474	A2	20020523	WO 2001-FR3559	20011114
WO 2002040474	A3	20021031		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2816618	A1	20020517	FR 2000-14738	20001115
FR 2816618	B1	20021227		
AU 2002018365	A5	20020527	AU 2002-18365	20011114
US 2002111492	A1	20020815	US 2001-987386	20011114
US 6603005	B2	20030805		
EE 200300207	A	20030815	EE 2003-207	20011114
EP 1337529	A2	20030827	EP 2001-996538	20011114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001015312	A	20030923	BR 2001-15312	20011114
JP 2004514661	T2	20040520	JP 2002-543484	20011114
NO 2003002187	A	20030626	NO 2003-2187	20030514

PRIORITY APPLN. INFO.: FR 2000-14738 A 20001115
US 2000-255145P P 20001214
WO 2001-FR3559 W 20011114
OTHER SOURCE(S): MARPAT 136:386033
GI

L5 ANSWER 2 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)



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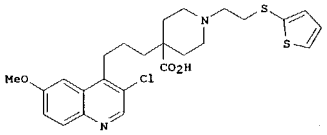
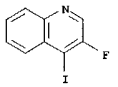


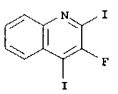
II

AB The invention concerns heterocyclylalkyl piperidine derivs. I, including their enantiomeric or diastereoisomeric forms, or mixts. thereof, and/or their syn or anti forms, or mixts. thereof, and their salts [wherein X1, X2, X3, X4, and X5 = C(R'1), C(R'2), C(R'3), C(R'4), C(R'5), or one of X-groups (at most) = N; R1, R'1, R'2, R'3, R'4, R'5 = H, halo, alkyl, cycloalkyl, Ph, PhS, OH, heterocyclyl, cyano, CO2H, alkoxycarbonyl, (un)substituted NH2, etc.; R2 = CO2H, alkyloxycarbonyl, cycloalkyloxycarbonyl, cyano, CONRaRb, CH2OH, substituted alkyl, CF2-Rc, C(CH3)2-Rc, CORc, CH(OH)-Rc, C(cycloalkyl)-Rc, or CH:CH-Rc; Ra, Rb = H, alkyl, cycloalkyl, Ph, heterocyclyl; or NRaRb = (un)substituted 5- or 6-membered heterocycle; Rc = CO2H, alkoxycarbonyl, cycloalkoxycarbonyl, CONRaRb; R3 = Ph, heterocyclyl, various substituted alkyls; Y = CH(Re), CF2, C(:NOH), alkyloxyiminomethylene, cycloalkyloxyiminomethylene, or C3-6 cycloalkylidene; Re = H, F, OH, alkoxy, cycloalkoxy, CO2H, alkoxycarbonyl, NRaRb, CONRaRb; and n = 0-4; wherein the radicals or Ph or heterocyclyl portions mentioned above can optionally be substituted]. Approx. 60 compds. were prepd., 5 were specifically claimed, and many more names were listed. For instance, Pd-complex-catalyzed coupling of 4-allyl-4-Cbz-1-BOC-piperidine with 4-bromo-3-chloro-6-methoxyquinoline (prepns. of both compds. given), followed by removal of the BOC group with CF3CO2H, N-alkylation with 2-[(2-bromoethyl)thio]thiophene, and hydrolysis of the benzyl ester (Cbz) in aq. HCl, gave title compd. II as the di-HCl salt. I are active against both gram-pos. and gram-neg. bacteria. I were active against exptl. infection of mice with Staphylococcus aureus IP8203 at 18-150 mg/kg s.c., or 20-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).
IT **213772-63-5P**, 3-Fluoro-4-iodoquinoline
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**

L5 ANSWER 2 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
(Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of quinolinylpropylpiperidinecarboxylic acids as antibacterials.)
RN 213772-63-5 CA
CN Quinoline, 3-fluoro-4-iodo- (9CI) (CA INDEX NAME)

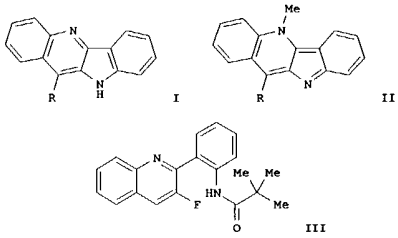


L5 ANSWER 3 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
structure-activity relationships. For benzo-.delta.-carbolines, methylation at N-5 increases the cytotoxic and antiparasitic activities. A further alkylation on C-11 generally increases the cytotoxic activity but not the antiparasitic activity, cryptolepine and 11-methylcryptolepine being the most active on both parasites. Taking advantage of the fluorescence of the indoloquinoline chromophore, cryptolepine was localized by fluorescence microscopy in parasite DNA-contg. structures suggesting that these compds. act through interaction with parasite DNA as proposed for cryptolepine on melanoma cells. For .delta.-carbolines, methylation at N-1 is essential for the antimalarial activity. 1-Methyl-.delta.-carboline specifically accumulates in the intracellular parasite. It has weak cytotoxic activity and can be considered as a potential antimalarial compd.
IT **213772-72-6P**
RL: RCT (Reactant); **PREP (Preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(cytotoxicity and antiplasmodial/antitrypanosomal activities of benzo-.delta.-carbolines and cryptolepines prepd. via regioselective cross-coupling reactions)
RN 213772-72-6 CA
CN Quinoline, 3-fluoro-2,4-diiodo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 134:295759 CA
TITLE: New synthesis of benzo-.delta.-carbolines, cryptolepines, and their salts: in vitro cytotoxic, antiplasmodial, and antitrypanosomal activities of .delta.-carbolines, benzo-.delta.-carbolines, and cryptolepines
AUTHOR(S): Arzel, Erwan; Rocca, Patrick; Grellier, Philippe; Labaeied, Mehdi; Frappier, Francois; Gueritte, Francoise; Gaspard, Christiane; Marsais, Francis; Godard, Alain; Queguiner, Guy
CORPORATE SOURCE: UMR 6014, Institut National des Sciences Appliquees, Mont-Saint-Aignan, 76131, Fr.
SOURCE: Journal of Medicinal Chemistry (2001), 44(6), 949-960
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:295759
GI



AB Benzo-.delta.-carbolines I and cryptolepines II (R = H, Me, Et, Pr, Ph) and their salts were prepd. using strategies based on the assocn. between halogen-dance and hetero-ring cross-coupling. The syntheses are fully convergent and regioselective with overall yields of 27-70%. Thus, coupling of 3-fluoro-2-iodoquinoline with the phenylboronate 2-(Me3CCONH)C6H4B(OH)2 gave the phenylquinoline III. Treatment of III with pyridinium chloride at 215.degree. for 30 min and then with aq. NH3 gave 83% I (R = H). A halogen-dance mechanism in the quinoline series was proposed. The formal synthesis of potential antimalarial compds. and the first total synthesis of 11-isopropylcryptolepine was described. Cytotoxic activity against mammalian cells and activities against Plasmodium falciparum and Trypanosoma cruzi of benzo-.delta.-carbolines and .delta.-carbolines were evaluated in vitro to study the

L5 ANSWER 4 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 133:350151 CA
TITLE: Preparation of quinoline derivatives as inhibitors of MEK enzymes
INVENTOR(S): Gibson, Keith Hopkinson
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068199	A1	20001116	WO 2000-GB1698	20000503
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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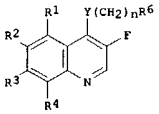
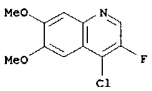
BR 2000010366	A	20020213	BR 2000-10366	20000503
EP 1178965	A1	20020213	EP 2000-927492	20000503
EP 1178965	B1	20030924		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200103185	T2	20020521	TR 2001-200103185	20000503
AT 250582	E	20031015	AT 2000-927492	20000503
US 6638945	B1	20031028	US 2001-959434	20011025
ZA 2001008969	A	20030130	ZA 2001-8969	20011030
NO 2001005447	A	20011212	NO 2001-5447	20011107

PRIORITY APPLN. INFO.: GB 1999-10580 A 19990508
WO 2000-GB1698 W 20000503
OTHER SOURCE(S): MARPAT 133:350151
GI



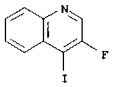
AB The title compds. I [n = 0-1; Y = NH, O, S, NR7 where R7 is alkyl of 1-6 carbon atoms; R6 = cycloalkyl, pyridinyl, pyrimidinyl, Ph; or R6 is a group R8XR9 and X is selected from CH2, NH, O, S, NR5; R1, R2, R3, R4 = H, OH, halo, cyano, NO2, etc.], inhibitors of MEK enzymes, were prepd. E.g.,

L5 ANSWER 4 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
reaction of 4-chloro-6,7-dimethoxy-3-fluoroquinoline (prepn. given) and 4-(2-methoxyphenoxy)aniline gave 4-(2-methoxyphenoxy)anilino-3-fluoro-6,7-dimethoxyquinoline.
IT **205448-48-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of quinoline derivs. as inhibitors of MEK enzymes)
RN 205448-48-2 CA
CN Quinoline, 4-chloro-3-fluoro-6,7-dimethoxy- (9CI) (CA INDEX NAME)



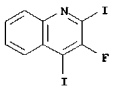
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 5 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 132:3495 CA
TITLE: First total synthesis of cryptomisrine
AUTHOR(S): Arzel, Erwan; Rocca, Patrick; Marsais, Francis; Godard, Alain; Queguiner, Guy
CORPORATE SOURCE: UPRES-A 6014 - IRCOF/INSA de Rouen, Mont Saint Aignan, 76131, Fr.
SOURCE: Tetrahedron (1999), 55(41), 12149-12156
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:3495
AB The first total synthesis of cryptomisrine, a novel indolo[3,2-b]quinoline dimeric alkaloid from Cryptolepis sanguinolenta, is reported. The approach is based on a convergent methodol. which involves a new halogen-dance reaction in 3-fluoro-4-iodoquinoline followed by its cross-coupling reaction to give bis-2-iodo-3-fluoroquinolin-4-ylmethanol which couples with 2-pivaloylaminophenylboronic acid and then heterocyclizes to cryptomisrine.
IT **213772-63-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(total synthesis of cryptomisrine)
RN 213772-63-5 CA
CN Quinoline, 3-fluoro-4-iodo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 6 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 129:276078 CA
TITLE: First halogen-dance reaction in quinoline series: application to a new synthesis of quindoline
AUTHOR(S): Arzel, Erwan; Rocca, Patrick; Marsais, Francis; Godard, Alain; Queguiner, Guy
CORPORATE SOURCE: UPRESA 6014 CNRS - IRCOF/INSA de Rouen, Mont Saint Aignan, 76131, Fr.
SOURCE: Tetrahedron Letters (1998), 39(36), 6465-6466
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:276078
AB The first halogen-dance reaction in the quinoline series is described and was applied to a new convergent synthesis of quindoline, a natural benzo-.delta.-carboline.
IT **213772-72-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(halogen-dance reaction in quinolines)
RN 213772-72-6 CA
CN Quinoline, 3-fluoro-2,4-diiodo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 7 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 128:270546 CA
TITLE: Quinoline derivatives inhibiting the effect of growth factors such as VEGF
INVENTOR(S): Thomas, Andrew Peter; Hennequin, Laurent Francois Andre; Ple, Patrick Alan
PATENT ASSIGNEE(S): Zeneca Ltd., UK; Zeneca Pharma S.A.; Thomas, Andrew Peter; Hennequin, Laurent Francois Andre; Ple, Patrick Alan
SOURCE: PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9813350	A1	19980402	WO 1997-GB2587	19970923
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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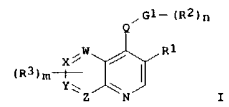
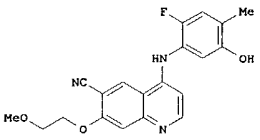
AU 9743137	A1	19980417	AU 1997-43137	19970923
AU 733551	B2	20010517		
EP 929526	A1	19990721	EP 1997-941115	19970923
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1237963	A	19991208	CN 1997-199929	19970923
JP 2001500890	T2	20010123	JP 1998-515386	19970923
NO 9901423	A	19990511	NO 1999-1423	19990324
KR 2000048575	A	20000725	KR 1999-702502	19990324

PRIORITY APPLN. INFO.: EP 1996-402034 A 19960925
WO 1997-GB2587 W 19970923
OTHER SOURCE(S): MARPAT 128:270546
GI

L5 ANSWER 7 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)



I



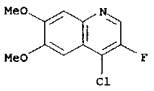
II

AB The invention relates to the use of compds. I [R1 = F or H; R2 = OH, halo, C1-3 alkyl, C1-3 alkoxy, C1-3 alkanoyloxy, CF3, cyano, amino, or NO2; n = 0-5; Q = O, NH, S, or CH2; G1 = Ph or 5- to 10-membered heteroarom. cyclic or bicyclic contg. O, S, and/or N; W, X, Y, Z = CH or N (but all 4 .noteq. N); m = 1-3; R3 = H, OH, halo, cyano, NO2, CF3, C1-3 alkyl, NR4R5 (wherein R4 and R5 = H or C1-3 alkyl), or R6X1- wherein X1 = CH2 or heteroatom linker group, and R6 = alkyl, alkenyl or alkynyl chain (un)substituted by OH, amino, NO2, alkyl, cycloalkyl, alkoxyalkyl, (un)substituted pyridone, Ph, heterocyclyl, etc. (which alkyl, alkenyl or alkynyl chain may have heteroatom linker), or R6 = (un)substituted pyridone, Ph, or heterocyclyl], and salts thereof, in the manuf. of medicaments for prodn. of an antiangiogenic and/or vascular permeability-reducing effect. Also disclosed are processes for the prepn. of I, and pharmaceutical compns. contg. them as active ingredients. I and salts inhibit the effects of VEGF, a property useful in the treatment of a no. of disease states including cancer and rheumatoid arthritis (no data). Examples include 63 syntheses and 7 general formulations. For instance, condensation of 4-chloro-6-cyano-7-(2-methoxyethoxy)quinoline hydrochloride with 2-fluoro-5-hydroxy-4-methylaniline (prepns. given) in refluxing iso-PrOH gave 68% title compd. II, isolated as the HCl salt.

IT **205448-48-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; prepn. of quinoline derivs. as growth factor inhibitors)

RN 205448-48-2 CA
CN Quinoline, 4-chloro-3-fluoro-6,7-dimethoxy- (9CI) (CA INDEX NAME)

L5 ANSWER 7 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

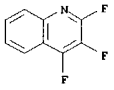
Exempted

L5 ANSWER 8 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 127:346280 CA
TITLE: Reactions of trifluorovinyllithium and 1-chloro-2,2-difluorovinyllithium: the synthesis of fluorinated heterocycles
AUTHOR(S): Burdon, J.; Coe, P. L.; Haslock, I. B.; Powell, R. L.
CORPORATE SOURCE: School of Chemistry, The University, Edgbaston, Birmingham, B15 2TT, UK
SOURCE: Journal of Fluorine Chemistry (1997), 85(2), 151-153
CODEN: JFLCAR; ISSN: 0022-1139
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Trifluorovinyllithium (from 1,1,1,2-tetrafluoroethane [HFC-134a]) reacted with 2-trifluoromethylaniline at -78 .degree.C to give 2,3,4-trifluoroquinoline in moderate to good yield. In a similar reaction, 1-chlorodifluorovinyllithium (from 1-chloro-2,2,2-trifluoroethane [HCFC-133a]) yielded 3-chloro-2,4-difluoroquinoline.

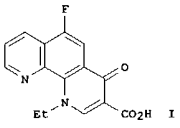
IT **198128-72-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of fluorinated heterocycles)

RN 198128-72-2 CA
CN Quinoline, 2,3,4-trifluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 9 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 122:133124 CA
TITLE: Quinolone(II):synthesis of fluoro-substituted pyrido[3,2-h]quinolone derivatives as potential antibacterials
AUTHOR(S): Lee, Jae Keun; Chang, Sha Joung
CORPORATE SOURCE: Dep. Chem., Coll. Natl. Sci., Taegu, 702-701, S. Korea
SOURCE: Korean Journal of Medicinal Chemistry (1994), 4(2), 92-100
CODEN: KJMCE7; ISSN: 1225-0058
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

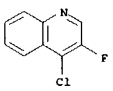


I

AB The potential antimicrobials, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-1,10-phenanthroline-3-carboxylic acid (I), 1-ethyl-1,4-dihydro-9-(4-methyl-1-piperazinyl)-4-oxo-1,10-phenanthroline-3-carboxylic acid and 1-ethyl-6-fluoro-1,4-dihydro-9-(4-methyl-1-piperazinyl)-4-oxo-1,10-phenanthroline-3-carboxylic acid were synthesized and their antibacterial activities were evaluated.

IT **161038-28-4P**, 4-Chloro-3-fluoroquinoline
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of bactericides 4-oxo-1,10-phenanthroline-3-carboxylates)

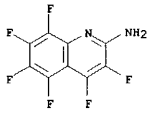
RN 161038-28-4 CA
CN Quinoline, 4-chloro-3-fluoro- (9CI) (CA INDEX NAME)



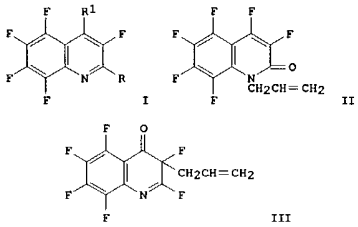
L5 ANSWER 10 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 120:134243 CA
TITLE: Remarkable orientational effects in the displacement of the fluorine from heptafluoroisoquinoline and -quinoline towards sulfur nucleophiles. Further reactions with oxygen nucleophiles
AUTHOR(S): Brooke, Gerald M.; Chambers, Richard D.; Drury, Christopher J.; Bower, Michael J.
CORPORATE SOURCE: Chem Dep., Sci. Lab., Durham, DH1 3LE, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1993), (18), 2201-9
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 1,3,4,5,6,7,8-Heptafluoroisoquinoline (I) and 2,3,4,5,6,7,8-heptafluoroquinoline (II) have been treated with a variety of sulfur and oxygen nucleophiles and some reactivities have been measured relative to treatment with ethoxide. The significant feature is that the major sites of attack by the sulfur and the oxygen nucleophiles are significantly different: attack occurs at the 6-position by sulfur and the 1-position by oxygen nucleophiles in the isoquinoline deriv. I irresp. of the relative reactivities; and at the 4-position by sulfur and at both the 2- and 4-positions by oxygen nucleophiles in the quinoline deriv. II. The results have been rationalized on the basis of the relative hardness/softness of the nucleophiles and the known activating influences of the fluorine atoms at sites remote from the reaction center.

IT **13180-57-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 13180-57-9 CA
CN 2-Quinolinamine, 3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)



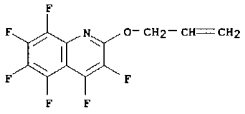
L5 ANSWER 11 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 110:38848 CA
TITLE: The preparation and thermolysis reactions of allyl 3,4,5,6,7,8-hexafluoroquinolin-2-yl ether, allyl 2,3,5,6,7,8-hexafluoroquinolin-4-yl ether and allyl 3,4,5,6,7,8-hexafluoroisoquinolin-1-yl ether
AUTHOR(S): Brooke, G. M.; Eggleston, I. M.; Hale, F. A.
CORPORATE SOURCE: Chem. Dep., Sci. Lab., Durham, DH1 3LE, UK
SOURCE: Journal of Fluorine Chemistry (1988), 38(3), 421-34
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:38848
GI



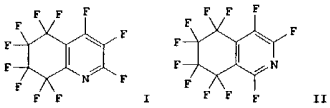
AB Reaction of CH2:CHCH2ONa with 2,3,4,5,6,7,8-heptafluoroquinoline gave 67 and 20% of ethers I (R = CH2:CHCH2O, R1 = F; R = F, R1 = CH2:CHCH2O), resp. Thermolysis of I (R = CH2:CHCH2O, R1 = F) in tetralin at 212.degree. for 48 h gave 69% of the Claisen rearrangement product II in which N is the migration terminus. However, a similar rearrangement of I (R = F, R1 = CH2:CHCH2O) in o-xylene at 147.5.degree. for 2.5 h gave allylquinolinone III, the product with C as the migration terminus.

IT **118097-74-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and Claisen rearrangement of)
RN 118097-74-8 CA
CN Quinoline, 3,4,5,6,7,8-hexafluoro-2-(2-propenyloxy)- (9CI) (CA INDEX NAME)

L5 ANSWER 11 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)

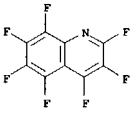


L5 ANSWER 12 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 107:23214 CA
TITLE: Polyhalogenoheterocyclic compounds. Part 37. Perfluorotetrahydroquinoline, -isoquinoline, and related compounds
AUTHOR(S): Bell, S. L.; Chambers, R. D.; Daniels, R.; Holmes, T. F.; Silvester, M. J.
CORPORATE SOURCE: Dep. Chem., Univ. Sci. Lab., Durham, DH1 3LE, UK
SOURCE: Journal of Fluorine Chemistry (1986), 32(4), 403-14
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:23214
GI

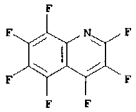


AB The formation of perfluorotetrahydroquinoline (I) and -isoquinoline II in the high temp. reaction between KF and heptachloroquinoline and -isoquinoline is investigated and a mechanism is proposed. I and II represent unusually substituted pyridine derivs. and the orientation of substitution in reactions with nucleophiles is reported.

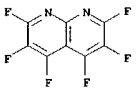
IT **13180-38-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and fluorination or chlorination of)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



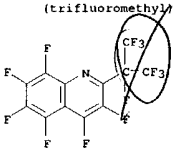
L5 ANSWER 13 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 84:135440 CA
TITLE: Perfluorodicarboxylic acids, VI. Preparation of perfluoropyridine-2,3-dicarboxylic acid by oxidation of perfluoroquinoline
AUTHOR(S): Sartori, P.; Ahlers, K.; Frohn, H. J.
CORPORATE SOURCE: Fachber. Chem., Gesamthochsch. Duisburg, Duisburg, Fed. Rep. Ger.
SOURCE: Journal of Fluorine Chemistry (1976), 7(4), 363-74
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: German
AB The oxidn. of perfluoroquinoline with 98% HNO3 yields perfluoropyridine-2,3-dicarboxylic acids, 2,3,4,6,7-pentafluoro-5,8-dioxo-5,8-dihydroquinoline, and 3,4,5,6,7,8-hexafluoro-2-oxo-1,2-dihydroquinoline.
IT **13180-38-6P**
RL: RCT (Reactant); **PREP (Preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and oxidn. of)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



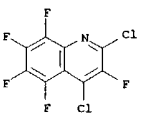
L5 ANSWER 14 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 83:131494 CA
TITLE: Preparation of hexafluoro-1,8- and -2,7-naphthyridine
AUTHOR(S): Van den Ham, D. M. W.
CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
SOURCE: Journal of Fluorine Chemistry (1975), 5(6), 537-44
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Hexachloro-1,8-(I) and -2,7-naphthyridine (II) were prepd. from 2,7-dichloro-1,8-naphthyridine and 1,3,6,8-tetrachloro-2,7-naphthyridine resp. From I and II and their starting materials a series of partially and totally fluorine substituted compds. were prepd.
IT **56595-12-1P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 56595-12-1 CA
CN 1,8-Naphthyridine, 2,3,4,5,6,7-hexafluoro- (9CI) (CA INDEX NAME)



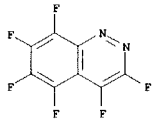
L5 ANSWER 15 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 77:19504 CA
TITLE: Reactions involving fluoride ion. V. Synthesis of perfluoro(isopropylquinolines)
AUTHOR(S): Chambers, R. D.; Corbally, R. P.; Musgrave, W. K. R.; Jackson, J. A.; Matthews, R. S.
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1972), (9-10), 1286-90
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB F-induced reaction of F3CCF:CF2 with perfluoroquinoline in triglyme or tetraglyme gave a mixt. of perfluoro(isopropylquinolines) [e.g. perfluoro(2,4-diisopropylquinoline) (I)], substitution occurring preferentially at the 2- and 4-positions followed by attack at the 6-position. I rearranged on heating with F-, giving the 2,6-isomer as the main product. Unusually large coupling consts. between a 4-(CF3)2CF group and a 5-F atom were obsd. in the 19F NMR spectra of these compds.; the temp. dependence of the spectra was discussed in terms of preferential population of particular conformations.
IT **36779-48-3P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 36779-48-3 CA
CN Quinoline, 3,4,5,6,7,8-hexafluoro-2-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 16 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 74:53453 CA
TITLE: Polyfluoroheterocyclic compounds. XVIII. Reactions of heptafluoroquinoline and -isoquinoline and pentafluoropyridine with hydrogen halides
AUTHOR(S): Chambers, Richard D.; Hole, M.; Musgrave, William K. R.; Thorpe, J. G.
CORPORATE SOURCE: Sci. Lab., Univ. Durham, Durham, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (1), 61-7
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB When pentafluoropyridine (I), heptafluoroquino-line (II), and heptafluoroisoquinoline (III) reacted with hydrogen halides in tetrahydrothiophene dioxide, F ortho and para to ring N was replaced by the other halogen. The order of reactivity is II >>> III >I. Reaction of II occurred at room temp. with substitution first at the 2- and than at the 4-position, to give 28-61% 2,4-dihalo derivs. Reaction of I or III required elevated temps.; I gave 4- and 2,4,6-substituted derivs., and III the 1-halo deriv. in low yields. Small amounts of H2O in the solvent deactivated the system. The mechanism of the reactions is discussed in terms of nucleophilic displacement of fluoride ion from the protonated species.
IT **27401-84-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 27401-84-9 CA
CN Quinoline, 2,4-dichloro-3,5,6,7,8-pentafluoro- (8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 17 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 73:66535 CA
TITLE: Hexafluorocinnoline: synthesis and photochemical isomerization to hexafluoroquinazoline
AUTHOR(S): Chambers, Richard D.; MacBride, John A. H.; Musgrave, William K. R.
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
SOURCE: Journal of the Chemical Society [Section] D: Chemical
Communications (1970), (12), 739-40
CODEN: CCJDAO: ISSN: 0577-6171
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Hexafluorocinnoline (I) was prepd. from hexachlorocinnoline (II) and isomerized to hexafluoroquinazoline (III) in 5-10% yields by uv irradn. at
.apprx.100.degree.. Thus, treating IV with SO2Cl2 and Ac2O in AcOH gave V; treating V with PCl5 in POCl3 gave VI; and treating VI with Cl and AlCl3 gave II, which was fluorinated with KF to give I and 5-chloropentafluorocinnoline. I reacted rapidly with atm. moisture to give VII and with NH3 to give VIII. Volatile products from I irradn. were
treated with aq. NH3 to give VIII, IX, and minor unidentified products. After irradn. of III for half the time of the I expt., 80% III was recovered with an involatile tar. I isomerization to III probably occurs via the benzodiazabenzvalene X.
IT **28734-86-3P**
RL: RCT (Reactant); **PREP (Preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and photochem. rearrangement of)
RN 28734-86-3 CA
CN Cinnoline, hexafluoro- (8CI, 9CI) (CA INDEX NAME)

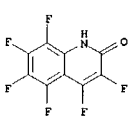


L5 ANSWER 18 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 71:81210 CA
TITLE: Heptafluoroquinoline and derivatives
INVENTOR(S): Chambers, Richard D.; Hole, Michael; Musgrave, William
K. R.
PATENT ASSIGNEE(S): National Research Development Corp.
SOURCE: Brit., 7 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1155965		19690625	GB	19650513

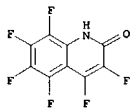
GI For diagram(s), see printed CA Issue.
AB The title compds. are prepd. Thus, an intimate mixt. of 31 g. heptachloroquinoline [m. 155-7.degree. (benzene), prepd. in 78% yield from
95.5 g. tetra-chloroquinoline and 1054 g. PCl5 at 315-30.degree.] and 72.5
g. anhyd. KF is heated 17 hrs. at 470.degree. in vacuo to give 18 g. of a
mixt. of 85% heptafluoroquinoline (I), b. 205-5.5.degree., m. 95-5.5.degree.; 12% chlorohexafluoroquinoline isomer (II), m. 89-90.degree.; and 3% isomer of II. A soln. of 0.1 g. Na in dry MeOH is added slowly to a stirred mixt. of 1.14 g. I in 12 ml. dry MeOH, and the mixt. stirred 15 min. and worked up to give 0.91 g. of a mixt. of 97% methoxyhexafluoroquinolines [3.4:1 mixt. of IIIa-IIIb (defined below)], 2%
I, and 1% 2,4-dimethoxy-3,5,6,7,8-pentafluoro-quinoline (IV), m. 107.5-8.5.degree. (MeOH), sepd. to give 2-methoxy-3,4,5,6,7,8-hexafluoroquinoline (IIIa), m. 50.5-1.5.degree., and 4-methoxy-2,3,5,6,7,8-
hexafluoroquinoline (IIIb), m. 68.5-69.degree.; similar expts. with other proportions of Na give IIIa, IV, and (probably) a >9:1 mixt. of 2,4,7- and
2,4,6-trimethoxytetra-fluoroquinolines, glassy at 123-35.degree., m. 135-6.degree.. A soln. of 1.28 g. N2H4.H2O in 5 ml. dioxane is added over
35 min. to a stirred soln. of 30.9 g. I in 20 ml. dioxane at 20.degree., and the mixt. stirred 45 min. and worked up to give 2.95 g. solid, sublimed in vacuo to give 76% 2-hydrazino-3,4,5,6,7,8-hexafluoroquinoline (V), decompd. 196.degree.. A soln. of 3.85 g. CuSO4.5H2O (VI) in 70 ml. H2O is added slowly over 45 min. to a suspension of 2.22 g. V in 50 ml. H2O, a soln. of 1.2 g. VI in 10 ml. H2O added, and the mixt. refluxed 1 hr. and worked up to give 0.5 g. solid, sublimed at 20-30.degree./0.1 mm. to give 3,4,5,6,7,8-hexafluoroquinoline, m. 62.5-4.5.degree.. Aq. NH3 (sp. gr. 0.88) (1 ml.) is added to a stirred soln. of 1 g. I in 10 ml. Me2CO at 20.degree., and the mixt. stirred 45 min. and worked up to give 0.9 g. solid, recrystd. (Me2CO-CH2Cl2) and sublimed in vacuo to give 2-amino-3,4,5,-6,7,8-hexafluoroquinoline (VII), m. 224-5.degree., and a 1:4 mixt., m. 158.5-60.degree., of VII and 4-amino-2,3,5,6,7,8-hexafluoroquinoline. A mixt. of 1.25 g. IV and 15 ml. 54% aq. HI is

L5 ANSWER 18 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
refluxed 5.5 hrs. and worked up to give 0.5 g. 2-hydroxy-4-methoxy-3,5,6,7,8-pentafluoroquinoline (VIII), m. 250-63.degree. (decompn.) (CHCl3-benzene), and 0.25 g. 2,4-dihydroxy-3,5,6,7,8-penta-fluoroquinoline
(IX), m. 245-55.degree. (decompn.) (EtOAc). A mixt. of 1 g. IIIa and 1.1 g. anhyd. AlCl3 is heated 3.5 hrs. at 120.degree. and worked up to give 0.5 g. 2-hydroxy-3,4,5,6,7,8-hexafluoroquinoline (X), m. 211.degree. (decompn.) (petroleum ether-CH2Cl2); a similar demethylation of IIIb with AlCl3 gives a mixt. (m. 137.5-9.5.degree. (decompn.), after sublimation at
80%/0.05 mm.) contg. 80% 4-hydroxy-2,3,5,6,7,8-hexafluoroquinoline. To a soln. of 1 g. I in 20 ml. H2SO4 (sp. gr. 1.84) is added dropwise 100 ml. H2O over 0.5 hr., and the ppt. (0.8 g.) filtered off and sublimed at 110.degree./0.1 mm. to give X. Excess CH2N2 in dry Et2O is added to a suspension of 2.35 g. IX in 300 ml. dry Et2O, and the mixt. worked up to give 2.1 g. of a 9:10 mixt., sepd. by fractional sublimation and recrystn., of IV and 4-methoxy-1-methyl-3,5,6,7,8-pentafluoro-2(1H)-quinolone (XI), m. 115-16.degree.; IV and XI are also obtained in a 4:5 ratio by similarly methylating VIII, while X gives IIIa and 1-methyl-3,4,5,6,7,8-hexafluoro-2(1H)-quinolone (XII), m. 127-7.4.degree.,
in 2:3 ratio. A stirred mixt. of 2 g. I and 0.88 g. KOH in 50 ml. H2O is refluxed 4.25 hrs., and worked up via CH2N2 to give 1.4 g. of a mixt. of 30% IIIa, 20% IIIb and 50% XII; an analogous reaction in Me3COH gives a mixt. of 32% IIIa, 6% IIIb, and 62% XII with the same amt. of KOH, and a mixt. of 40% IIIa, 2% IIIb, 38% XII, 15% IV, and 5% XI with half again the
amt. KOH. MeOH (150 ml.) is added dropwise over 1 hr. to a soln. of 1 g. I in 20 ml. H2SO4 (sp. gr. 1.84) at 0.degree., the soln. shaken with CH2Cl2, 150 ml. H2O added slowly over 1 hr., and the mixt. worked up to give 0.55 g. of a 3:17 mixt. of I and IIIa, and 0.1 g. X.
IT **13180-42-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 13180-42-2 CA
CN 2(1H)-Quinolinone, 3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)

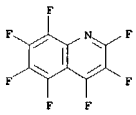


L5 ANSWER 19 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 70:11541 CA
TITLE: Synthetic nucleosides and nucleotides. V. Synthesis and reaction of 3-fluoro-4-nitroquinoline 1-oxide
AUTHOR(S): Araki, Misako; Saneyoshi, Mineo; Harada, Harue; Kawazoe, Yutaka
CORPORATE SOURCE: Nat. Cancer Center Res. Inst., Tokyo, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1968), 16(9), 1742-6
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 70:11541
GI For diagram(s), see printed CA Issue.
AB 3-Fluoroquinoline 1-oxide, which was prepd. through the Schiemann reaction
of 3-aminoquinoline, followed by N-oxygenation, was nitrated to 3-fluoro-4-nitroquinoline 1-oxide (I). The fluorine atom of I was replaced with nucelophiles such as OR- or NR2-contg. compds. in neutral or
alk. media to afford 3-substituted 4-nitroquinoline 1-oxide derivs. The reaction with aq. HCl brought about the replacement of the nitro group to give 3-fluoro-4-chloroquinoline 1-oxide.
IT **20849-68-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 20849-68-7 CA
CN Quinoline, 4-chloro-3-fluoro-, 1-oxide (8CI) (CA INDEX NAME)

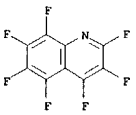
L5 ANSWER 20 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 66:46302 CA
TITLE: Polyfluoroheterocyclic compounds. IX. Tautomerism in polyfluorohydroxyquinolines and -isoquinolines
AUTHOR(S): Chambers, Richard D.; Hole, Michael; Musgrave, William K. R.; Storey, R. A.
CORPORATE SOURCE: Univ. Sci. Labs., Durham, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1967), (1), 53-7
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cf. CA 66, 28627w. Heptafluoroquinoline with aq. NaOH or with KOH in tert-BuOH gives a mixt. of 2-and 4-hydroxyhexafluoroquinolines; heptafluoroisoquinoline reacts to give the 1-hydroxy deriv. 2-Hydroxyhexafluoroquinoline (I) and 1-hydroxyhexafluoroisoquinoline exist as tautomers and react with CH2N2 giving a mixt. of O-and N-Me derivs. whereas 4-hydroxyhexafluoroquinoline gives only an O-Me deriv. The factors affecting tautomerism in these systems are outlined.
IT **13180-42-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 13180-42-2 CA
CN 2(1H)-Quinolinone, 3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)



L5 ANSWER 21 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 66:28627 CA
TITLE: Polyfluoro heterocyclic compounds. VIII. Nucleophilic substitution in heptafluoroquinoline and -isoquinoline
AUTHOR(S): Chambers, Richard D.; Hole, Michael; Musgrave, William K. R.; Storey, R. A.; Iddon, Brian
CORPORATE SOURCE: Univ. Sci. Labs., Durham, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1966), (24), 2331-9
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. preceding abstr. Nucleophilic substitution in heptafluoroquinoline and (or) heptafluoroisoquinoline by various nucleophiles, e.g., sodium methoxide, ammonia, hydrazine, and LiAlH4 is described. Monosubstitution and disubstitution in heptafluoroquinoline occurs at the 2-and 4-positions while in heptafluoroisoquinoline attack occurs first, specifically, at the 1-position and then at the 6-position. Oxidn. of heptafluoroisoquinoline and the methoxy derivs. gives tri- and difluoropyridinedicarboxylic acids which aid the analysis of the 19F N.M.R. spectra of the methoxy derivs. and establish their structures. Analysis of the 19F N.M.R. spectra of the derivs. of heptafluoroquinoline also clearly distinguishes their structures. In both series, some very large coupling consts. are observed which are assigned to peri F-F coupling. The major factor detg. the orientation of nucleophilic substitution in these systems is the effect of the ring nitrogen on the relative stabilities of the transition states.
IT **13180-38-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 22 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 66:28626 CA
TITLE: Polyfluoro heterocyclic compounds. VII. Heptafluoroquinoline and -isoquinoline
AUTHOR(S): Chambers, Richard D.; Hole, Michael; Iddon, Brian; Musgrave, William K. R.; Storey, R. A.
CORPORATE SOURCE: Univ. Sci. Labs., Durham, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1966), (24), 2328-31
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cf. CA 64, 7986c. Heptachloroquinoline and -iso-quinoline have been prepd. by initial direct chlorination of quinoline and isoquinoline and subsequent reaction of the products with PO5 at elevated temps. Reaction of these perchloro compds. with KF at elevated temps. gives heptafluoroquinoline (I) and -isoquinoline in good yields. The perhalo quinolines and isoquinolines show no basic properties except that they dissolve in concd. sulfuric acid, and that the soln. of heptafluoroquinoline on slow addn. of water or methanol gives the monohydroxy or -methoxy derivs. but on rapid dilu. gives heptafluoroquinoline. The mechanism of the reaction is discussed in terms of nucleophilic displacement of fluoride ion from the protonated species.
IT **13180-38-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



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L6 ANSWER 1 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 140:235614 CA
TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
INVENTOR(S): Bacque, Eric; Bigot, Antony; El Ahmad, Youssef; Malleron, Jean Luc; Mignani, Serge; Ronan, Baptiste; Tabart, Michel; Viviani, Fabrice
PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.
SOURCE: Fr. Demande, 66 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844270	A1	20040312	FR 2002-11212	20020911
WO 2004024712	A1	20040325	WO 2003-FR2686	20030910

W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, RO, SC, SG, SY, TN, TT, UA, UZ, VC, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

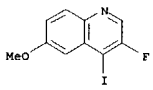
US 2004087619	A1	20040506	US 2003-659164	20030910

PRIORITY APPLN. INFO.: FR 2002-11212 A 20020911
OTHER SOURCE(S): MARPAT 140:235614
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H or F; R2 = COOH, CH2CO2H, CH2OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3 -7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = C1-6 alkyl, alkenyl-CH2, or alkynyl-CH2 (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including

L6 ANSWER 1 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
enantiomeric and diastereoisomeric forms, mixts. thereof, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Five synthetic examples are given. For example, II was prepd. by N-alkylation of III (prepn. given) with 2-[(2-bromoethyl)sulfanyl]-1,4-difluorobenzene, followed by acidic hydrolysis. Compds. I were active against exptl. infections of mice by Staphylococcus aureus IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).
IT **426842-84-4**, 4-Iodo-3-fluoro-6-methoxyquinoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of quinolylpropylpiperidines as antimicrobials)
RN 426842-84-4 CA
CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



IT **426842-84-4**, 4-Iodo-3-fluoro-6-methoxyquinoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of quinolylpropylpiperidines as antimicrobials)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 137:232568 CA
TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
INVENTOR(S): Bacque, Eric; Mignani, Serge; Malleron, Jean-Luc; Tabart, Michel; Evers, Michel; Viviani, Fabrice; El-Ahmad, Youssef; Mutti, Stephane; Daubie, Christophe
PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
SOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072572	A1	20020919	WO 2002-FR851	20020311

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

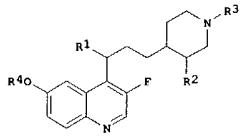
FR 2822154	A1	20020920	FR 2001-3374	20010313
EP 1370550	A1	20031217	EP 2002-722329	20020311

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 2002177606	A1	20021128	US 2002-96482	20020313
US 6602884	B2	20030805		
US 2003171369	A1	20030911	US 2003-387479	20030314

PRIORITY APPLN. INFO.: FR 2001-3374 A 20010313
US 2001-281407P P 20010405
WO 2002-FR851 W 20020311
US 2002-96482 A3 20020313
OTHER SOURCE(S): MARPAT 137:232568
GI

L6 ANSWER 2 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)



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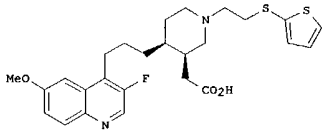
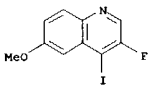


II

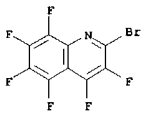
AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H, halo, OH, NH2, alkylamino, dialkylamino, hydroxyamino, alkoxyamino, or alkylalkoxyamino; R2 = COOH, CH2CO2H, CH2OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3 -7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = C1-6 alkyl, alkenyl-CH2, or alkynyl-CH2- (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including diastereoisomeric forms, mixts. thereof, cis or trans forms, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Ten synthetic examples are given. For instance, Wittig reaction of 4(RS)-4-allyl-1-(benzyloxycarbonyl)piperidin-3-one with Ph3P:CHCO2Me gave a Z-isomeric exocyclic olefin, which underwent hydroboration at allyl and Pd-catalyzed coupling with 4-iodo-3-fluoro-6-methoxyquinoline, followed by hydrogenation of the olefin with concomitant N-deprotection, N-alkylation with 2-(2-bromoethylthio)thiophene, and sapon. of the Me ester, to give the racemic title compd. II.2HCl. Compds. I were active against exptl. infections of mice by Staphylococcus aureus IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).
IT **426842-84-4**, 4-Iodo-3-fluoro-6-methoxyquinoline

L6 ANSWER 2 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
RL: RCT (Reactant); RACT (Reactant or reagent)
(precursor; prepn. of (quinolylpropyl)piperidine derivs. as antimicrobials)
RN 426842-84-4 CA
CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



IT **426842-84-4**, 4-Iodo-3-fluoro-6-methoxyquinoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(precursor; prepn. of (quinolylpropyl)piperidine derivs. as antimicrobials)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L6 ANSWER 3 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 137:62929 CA
TITLE: DFT Calculation of NMR JFF Spin-Spin Coupling Constants in Fluorinated Pyridines
AUTHOR(S): Barone, Veronica; Peralta, Juan E.; Contreras, Ruben H.; Snyder, James P.
CORPORATE SOURCE: Departamento de Fisica FCEyN, Universidad de Buenos Aires, Buenos Aires, Argent.
SOURCE: Journal of Physical Chemistry A (2002), 106(23), 5607-5612
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB All four isotropic contributions to the NMR fluorine-fluorine coupling consts. (Fermi contact, FC, spin-dipolar, SD, paramagnetic spin-orbit, PSO, and diamagnetic spin-orbit, DSO) have been calcd. for 2,6-difluoropyridine, 2,4,6-trifluoropyridine, perfluoropyridine, and 2-Br-3,4,5,6,7,8-hexafluoroquinoline by means of d. functional theory in combination with the rather modest 6-311G** basis set. Exptl. values ranging from -20.3 to +45.8 Hz are semiquant. reproduced for three- to seven-bond couplings, suggesting that the different electronic effects responsible for the spin-spin interactions are adequately taken into account. In all cases, the relative importance of noncontact terms was examd. With few exceptions, the sum of the SD and PSO noncontact terms is larger than the FC contact contribution, even though in most cases the two noncontact values have opposite signs. The widespread assumption that the Fermi contact term dominates scalar spin-spin couplings in the case of light atoms would appear to be an oversimplification for JFF in polyfluorinated org. mols. In addn., the CPU performance of the Fermi contact contribution calcd. sep. by the coupled-perturbed and the finite-perturbation methods was investigated showing the latter to be slightly more efficient.
IT **60870-78-2**, 2-Bromohexafluoroquinoline
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP
(Physical process); PROC (Process)
(DFT calcn. of NMR spin-spin coupling consts. in fluorinated pyridines)
RN 60870-78-2 CA
CN Quinoline, 2-bromo-3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)



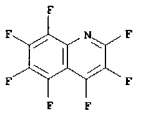
IT **60870-78-2**, 2-Bromohexafluoroquinoline

L6 ANSWER 3 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP
(Physical process); PROC (Process)
(DFT calcn. of NMR spin-spin coupling consts. in fluorinated pyridines)
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L6 ANSWER 4 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 119:206380 CA
TITLE: Extraction of perfluoroalkyl sulfonyl fluoride
INVENTOR(S): Sato, Yukio
PATENT ASSIGNEE(S): Tookemu Purodakutsu Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05168844	A2	19930702	JP 1991-65523	19910306
JP 3030661	B2	20000410		

PRIORITY APPLN. INFO.: JP 1991-65523 19910306
AB Perfluoroalkyl sulfonyl fluoride CnF2n+1SO2F (n=2-5) in F-contg. inert solvents is extd. by contacting with an aq. or alc. soln. contg. hydroxide or carbonate of alkali or alk. earth metals, preferably selected from KOH, NaOH, LiOH, Ba(OH)2, K2CO3, or Li2CO3.
IT **13180-38-6**, Perfluoroquinoline
RL: USES (Uses)
(extn. of perfluoroalkyl sulfonic fluoride from, by potassium hydroxide soln.)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)

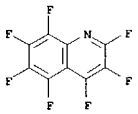


IT **13180-38-6**, Perfluoroquinoline
RL: USES (Uses)
(extn. of perfluoroalkyl sulfonic fluoride from, by potassium hydroxide soln.)

L6 ANSWER 5 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 119:206379 CA
TITLE: Separation of perfluoroalkyl sulfonyl fluoride
INVENTOR(S): Sato, Yukio
PATENT ASSIGNEE(S): Tookemu Purodakutsu Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

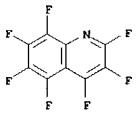
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05168843	A2	19930702	JP 1991-65517	19910306
JP 3030660	B2	20000410		

PRIORITY APPLN. INFO.: JP 1991-65517 19910306
AB A gas contg. perfluoroalkyl sulfonic fluoride (I) CnF2n+1SO2F (n=2-5) is contacted with a F-contg. inert solvent as an absorbent to sep. I. The gas contg. I is produced by electrolytic fluorination of alkyl sulfonic acid, alkylsulfonic fluoride, or alkylsulfonic chloride.
IT **13180-38-6**, Perfluoroquinoline
RL: USES (Uses)
(absorbent, sepn. of perfluoroalkyl sulfonic fluoride by, from reaction gas mixts.)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



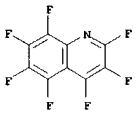
IT **13180-38-6**, Perfluoroquinoline
RL: USES (Uses)
(absorbent, sepn. of perfluoroalkyl sulfonic fluoride by, from reaction gas mixts.)

L6 ANSWER 6 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 95:167967 CA
TITLE: Proton-proton inter-ring coupling constants in isoquinoline and quinazoline. Their relationship with corresponding fluorine-19-fluorine-19 couplings in perfluoro derivatives
AUTHOR(S): Cassidei, L.; Sciacovelli, O.
CORPORATE SOURCE: Ist. Chim. Fis., Univ. Bari, Bari, 70126, Italy
SOURCE: Journal of Magnetic Resonance (1969-1992) (1981), 44(2), 340-7
CODEN: JOMRA4; ISSN: 0022-2364
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Complete spectral anal. of 1H NMR of isoquinoline and quinazoline is performed. Signs of interfering coupling consts. (JHHir) are detd. by INDOR expts. The mechanisms of transmission of JHHir are discussed. A linear correlation exists between the majority of JHHir of quinoline, isoquinoline, and quinazoline and JFFir of their perfluoro derivs.; exceptions are rationalized. The linear relationship, with the near-zero value of intercept, strongly suggests that JFFir originate, almost quant., from the Fermi contact term and are transmitted via the .pi.-electron system, except for the peri JFFir. A calcn. of the proportionality between JHHir and JFFir in quinoline, using the Pople and Santry expression for the contribution of .pi. electrons to interring coupling consts., agrees with the exptl. data.
IT **13180-38-6**
RL: PRP (Properties)
(interring proton coupling const. in quinoline vs.)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



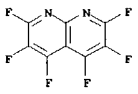
IT **13180-38-6**
RL: PRP (Properties)
(interring proton coupling const. in quinoline vs.)

L6 ANSWER 7 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 91:90752 CA
TITLE: Relationship between proton-proton and fluorine-19-fluorine-19 inter-ring coupling constants in fused aza aromatic systems
AUTHOR(S): Cassidei, L.; Dell'Atti, A.; Sciacovelli, O.
CORPORATE SOURCE: Ist. Chim. Fis., Univ. Bari, Bari, 70100, Italy
SOURCE: Spectroscopy Letters (1979), 12(5), 365-9
CODEN: SPLEBX; ISSN: 0038-7010
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Inter-ring coupling consts. (JFF and JHH) in quinoline, isoquinoline, and the corresponding perfluoro derivs. were detd. The data indicate that JFF are transmitted only through .pi.-electrons and large stereospecific .sigma.-contributions transmitted through the all-trans pathway are absent in F-F coupling.
IT **13180-38-6**
RL: PRP (Properties)
(fluorine-fluorine coupling consts. in)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



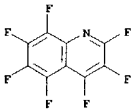
IT **13180-38-6**
RL: PRP (Properties)
(fluorine-fluorine coupling consts. in)

L6 ANSWER 8 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 91:67917 CA
TITLE: Rapid general microdetermination of fluorine
AUTHOR(S): Van Leuven, H. C. E.; Rotscheid, G. J.; Buis, W. J.
CORPORATE SOURCE: K./Shell Lab., Amsterdam, Neth.
SOURCE: Fresenius' Zeitschrift fuer Analytische Chemie (1979), 296(1), 36-9
CODEN: ZACFAU; ISSN: 0016-1152
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A rapid micromethod for the detn. of F in a wide variety of materials is based on the liberation of F as HF from the sample by means of pyrohydrolysis with steam at 1120.degree.. The amt. of F in the condensate is subsequently measured with an ion-selective electrode by using a simple std. addn. technique, which automatically compensates for variations in ionic strength, acidity, etc. Metals that may form stable complexes with fluoride are masked by the addn. of a complexing agent to the condensate. Materials analyzed included org. and organometallic compds., alumina-base catalysts, coal, etc. The limit of detection is of the order of 1 .mu.g F; the std. deviation is about 1% relative. The time required for one detn. is 15-20 min.
IT **56595-12-1**
RL: AMX (Analytical matrix); ANST (Analytical study)
(fluorine detn. in, by pyrohydrolysis and subsequent potentiometry)
RN 56595-12-1 CA
CN 1,8-Naphthyridine, 2,3,4,5,6,7-hexafluoro- (9CI) (CA INDEX NAME)



IT **56595-12-1**
RL: AMX (Analytical matrix); ANST (Analytical study)
(fluorine detn. in, by pyrohydrolysis and subsequent potentiometry)

L6 ANSWER 9 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 87:4858 CA
TITLE: Fluorine-19 NMR spectra of heptafluoroisoquinoline and hexafluoro-1-methoxyisoquinoline. Long-range inter-ring coupling constants
AUTHOR(S): Matthews, R. S.
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
SOURCE: Organic Magnetic Resonance (1976), 8(12), 628-31
CODEN: ORMRBD; ISSN: 0030-4921
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An anal. of the 19F NMR spectra of heptafluoroisoquinoline and hexafluoro-1-methoxyisoquinoline is presented. The inter-ring F-F coupling consts. alternate in sign and magnitude and are pos. over an odd no. of bonds. They correlated with SCFMO C-C polarizabilities inferring that the long-range coupling mechanism is dominated by the contribution from the .pi.-electron system.
IT **13180-38-6**
RL: PRP (Properties)
(bond polarizability and .pi.-bond order of, MO calcn. of)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



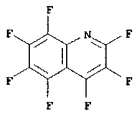
IT **13180-38-6**
RL: PRP (Properties)
(bond polarizability and .pi.-bond order of, MO calcn. of)

L6 ANSWER 10 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
(fluorine-19 NMR of)
IT **13180-38-6 27401-84-9 60870-78-2**
RL: PRP (Properties)
(fluorine-fluorine spin coupling consts. in)

L6 ANSWER 10 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 85:176425 CA
TITLE: Fluorine-19 NMR spectra of polyfluoroquinolines. Long range interring fluorine-19-fluorine-19 coupling constants and fluorine-19 chemical shifts
AUTHOR(S): Matthews, R. S.
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
SOURCE: Organic Magnetic Resonance (1976), 8(5), 240-5
CODEN: ORMRBD; ISSN: 0030-4921
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The signs and magnitudes of F-F coupling consts. in perfluoroquinoline (I), 2,4-dichloropentafluoroqinoline, and 2-bromohexafluoroquinoline were detd. by 19F NMR, providing unambiguous assignment of the spectra of I and derivs. Inter-ring F-F coupling consts. were pos. over an odd no. of bonds, and neg. over an even no. The 19F chem. shifts of I and I.F3CCO2H are reported and directly correlated with SCF MO calcd. .pi.-electron ds. at F and bonded C atoms.
IT **60870-79-3**
RL: PROC (Process)
(fluorine-19 NMR of)
RN 60870-79-3 CA
CN Quinoline, heptafluoro-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 13180-38-6
CMF C9 F7 N

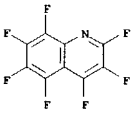


CM 2

CRN 76-05-1
CMF C2 H F3 O2

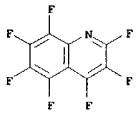
IT **60870-79-3**
RL: PROC (Process)

L6 ANSWER 11 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 84:4155 CA
TITLE: Electrochemical reduction of azaaromatics. V. Influence of fluorine substitution on the electron affinities
AUTHOR(S): Van den Ham, D. M. W.; Harrison, G. F. S.; Spaans, A.; Van der Meer, D.
CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1975), 94(7), 168-73
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The electrochem. redn. process of fluoro-substituted azaaromatics, e.g., 3,6-difluoropyridazine, is described by the pattern which is normally postulated for aryl halogenides, that is, fission of the C-halogen bond. However, the stability of the intermediate mononegative ions is generally higher than for the comparable fluoro-substituted arenes. As an example of this stability, the ERS spectrum of tetrafluoroquinoxaline is given. The half-wave redn. potentials of the first redn. wave are related to the electron affinities of the molecules. These electron affinities are correlated with those obtained by semi-empirical quantum chem. calcns.
IT **13180-38-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(electrochem. redn. of, electron affinity in relation to)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



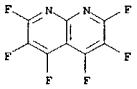
IT **13180-38-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(electrochem. redn. of, electron affinity in relation to)

L6 ANSWER 12 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 83:114335 CA
TITLE: Reactions involving fluoride ion. XII. Reactions of polyfluoro aromatic compounds with octafluorobut-2-ene
AUTHOR(S): Chambers, R. D.; Jackson, J. A.; Partington, S.; Philpot, P. D.; Young, A. C.
CORPORATE SOURCE: Dep. Chem., Univ. Sci. Lab., Durham, UK
SOURCE: Journal of Fluorine Chemistry (1975), 6(1), 5-18
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Octafluorobut-2-ene is much more difficult to dimerize, with fluoride ion, than is hexafluoropropene but perfluoro-3,4-dimethylhex-3-ene is obtained under more forcing conditions. Polyfluoroalkylations with octafluorobut-2-ene are very efficient and results with perfluoropyridine, -pyridazine, and -pyrimidine, and quinoline are described, giving various perfluoro-2-butyl derivs. Reactions with nitropentafluorobenzene and perfluorotoluene are also described. The 19F NMR spectra of perfluoro-2-butylaromatic compds. reveal restricted rotation, even at room temp.
IT **13180-38-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(perfluoroalkylation of, with octafluorobutene in presence of fluoride ion)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



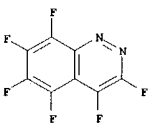
IT **13180-38-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(perfluoroalkylation of, with octafluorobutene in presence of fluoride ion)

L6 ANSWER 13 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 83:105955 CA
TITLE: Photoelectron spectra of fluorine substituted diazanaphthalenes. Even cases
AUTHOR(S): Van den Ham, D. M. W.; Beerlage, M.; Van der Meer, D.; Feil, D.
CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
SOURCE: Journal of Electron Spectroscopy and Related Phenomena
(1975), 7(1), 33-43
CODEN: JESRAW; ISSN: 0368-2048
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The high resolution He 584 .ANG. photoelectron spectra of 3 diazanaphthalenes and some of their fluoro derivs. are presented. The qualitative model that is used frequently in the discussion of lone-pair level splittings was examd.
IT **56595-12-1**
RL: PRP (Properties)
(uv photoelectron spectrum and ionization potential of)
RN 56595-12-1 CA
CN 1,8-Naphthyridine, 2,3,4,5,6,7-hexafluoro- (9CI) (CA INDEX NAME)



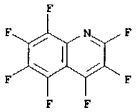
IT **56595-12-1**
RL: PRP (Properties)
(uv photoelectron spectrum and ionization potential of)

L6 ANSWER 14 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 80:2917 CA
TITLE: Photoelectron spectra of some fluorine substituted diazanaphthalenes
AUTHOR(S): Van den Ham, D. M. W.; Van der Meer, D.
CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
SOURCE: Journal of Electron Spectroscopy and Related Phenomena
(1973), 2(3), 247-58
CODEN: JESRAW; ISSN: 0368-2048
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The high resolution He 584 .ANG. photoelectron spectra of unsubstituted and fluorine-substituted 1,2-, 1,3-, 1,4- and 2,3-diazanaphthalenes are presented. F substitution enables more definite anal. of the photoelectron spectra of the parent compds. Unexpected shifts of the N lone-pair bands can be explained within the through-space and through-bond interaction model and it was deduced that F substitution can give exptl. evidence about the sym. character of the lone-pair MO.
IT **28734-86-3**
RL: PRP (Properties)
(photoelectron spectrum of)
RN 28734-86-3 CA
CN Cinnoline, hexafluoro- (8CI, 9CI) (CA INDEX NAME)



IT **28734-86-3**
RL: PRP (Properties)
(photoelectron spectrum of)

L6 ANSWER 15 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 77:132989 CA
TITLE: Perfluoro effect in the photoelectron spectra of quinoline and isoquinoline
AUTHOR(S): Van den Ham, D. M. W.; Van der Meer, D.
CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
SOURCE: Chemical Physics Letters (1972), 15(4), 549-52
CODEN: CHPLBC; ISSN: 0009-2614
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The high-resoln. He 584-.ANG. photoelectron spectra of heptafluoroquinoline and heptafluoroisoquinoline are compared with those of the parent compds. Shifts in .pi.-ionization potentials, due to the F substitution, can be described with an inductive and a combined inductive-conjugative Hueckel model.
IT **13180-38-6**
RL: PRP (Properties)
(photoelectron spectrum of, fluorine substitution effects in relation to)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)

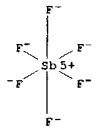


IT **13180-38-6**
RL: PRP (Properties)
(photoelectron spectrum of, fluorine substitution effects in relation to)

L6 ANSWER 16 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 75:117851 CA
TITLE: Polyfluoro-heterocyclic compounds. XIX. Relative base strengths of some polyfluoroaryl-nitrogen heterocyclic systems
AUTHOR(S): Bell, S. L.; Chambers, R. D.; Musgrave, W. K. R.; Thorpe, J. G.
CORPORATE SOURCE: Dep. Chem., Univ. Sci. Lab., Durham, UK
SOURCE: Journal of Fluorine Chemistry (1971), 1(1), 51-7
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of hexafluoroantimonate salts of perfluoropyridine, perfluoroquinoline, perfluoroisoquinoline, and perfluoropyrazine, and of 3,5-dichlorofluoropyridine were isolated. A relative order of base strength was obtained from 19F NMR measurements on mixts. of bases with acid which indicated that a dominant factor affecting base strength was the no. of F atoms ortho to the N atom.
IT **33808-40-1**
RL: PRP (Properties)
(basicity of, N.M.R. in relation to)
RN 33808-40-1 CA
CN Antimonate(1-), hexafluoro-, (OC-6-11)-, hydrogen, compd. with heptafluoroquinoline (1:1) (9CI) (CA INDEX NAME)

CM 1

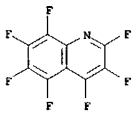
CRN 16950-06-4
CMF F6 Sb . H
CCI CCS



CM 2

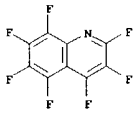
CRN 13180-38-6
CMF C9 F7 N

L6 ANSWER 16 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)



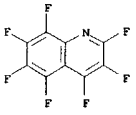
IT **33808-40-1**
RL: PRP (Properties)
(basicity of, N.M.R. in relation to)
IT **13180-38-6**
RL: PRP (Properties)
(nuclear magnetic resonance of)

L6 ANSWER 17 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 71:61301 CA
TITLE: Acid catalyzed nucleophilic substitutions in perfluoro
heterocyclic systems
AUTHOR(S): Musgrave, William K. R.
CORPORATE SOURCE: Univ. Durham, Durham, UK
SOURCE: Chemistry & Industry (London, United Kingdom) (1969), (28), 943-7
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Perfluoroquinoline (I) reacted with anhyd. HCl in dried sulfolane to give 2-chlorohexafluoroquinoline, 2,4-dichloro-pentafluoroquinoline, and 2-chloro-4-hydroxypentafluoroquino-line. The latter was absent when sulfolane dried over mol. sieves was used. HBr gave the corresponding products only when rigorously dry sulfolane was used. Very little substitution was shown by pentafluoropyridine treated with HCl and HBr as above; however, tetrafluoropyridazine (II) was more susceptible to nucleophilic substitution, the F in positions 4 and 5 reacting 1st, while in acid soln. 3-F and 6-F were replaced 1st. When HCl was bubbled through
II in Et2O, all 4-F atoms were replaced. AlCl3 and AlBr3 reacted with I at 150.degree. to give only 2-substituted products, but AlBr3 at >150.degree. and AlI3 at 150.degree. gave 2,8-disubstituted derivs. Pentafluoropyridine decompd. when heated with Al halides; however, when the corresponding halogen acid was added, the same products were obtained as in the reactions involving the halogen acid alone.
IT **13180-38-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, mechanism of)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT **13180-38-6 27401-84-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, mechanism of)

L6 ANSWER 18 OF 18 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 69:82102 CA
TITLE: Ground states of conjugated molecules. X. Fluorine-19 N.M.R. chemical shifts in aryl fluorides
AUTHOR(S): Dewar, Michael J. S.; Kelemen, Jozsef
CORPORATE SOURCE: Univ. of Texas, Austin, TX, USA
SOURCE: Journal of Chemical Physics (1968), 49(2), 499-508
CODEN: JCPSA6; ISSN: 0021-9606
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The procedures developed in previous papers of this series have been extended to aromatic fluorides, by using 19F N.M.R. chem. shifts as a guide to the selection of parameters for F. Attempts to correlate chem. shifts with the local .pi.-electron d. on F proved unsatisfactory, the correlation depending on the no. of atoms ortho to F that carry p or .pi. electrons. Similar results followed for charge ds. calcd. by a recently developed semiempirical self-consistent field M.O. treatment in which all the valence electrons are included. Anal. of the Karplus-Das-Prosser-Goodman treatment of chem. shifts suggested that this "ortho effect" arose
from neglected long-range interactions. A treatment including these was developed and shown to account well for the 19F chem. shifts of nearly 100
aryl fluorides.
IT **13180-38-6**
RL: PRP (Properties)
(nuclear magnetic resonance of, electron configuration in relation to)
RN 13180-38-6 CA
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT **13180-38-6 13323-16-5**
RL: PRP (Properties)
(nuclear magnetic resonance of, electron configuration in relation to)

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L2            2 S L1 SAM
L3           39 S L1 FULL

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L4           40 S L3
L5           22 S L3/PREP
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Executing the logoff script...


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STN INTERNATIONAL LOGOFF AT 15:53:57 ON 02 JUN 2004
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L5 ANSWER 1 OF 5 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 140:253457 CA
TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
INVENTOR(S): Bacque, Eric; Bigot, Antony; El Ahmad, Youssef; Malleron, Jean Luc; Mignani, Serge; Ronan, Baptiste; Tabart, Michel; Viviani, Fabrice
PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.
SOURCE: Fr. Demande, 96 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844268	A1	20040312	FR 2002-11213	20020911
WO 2004024713	A1	20040325	WO 2003-FR2687	20030910
W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, RO, SC, SG, SY, TN, TT, UA, UZ, VC, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004082610	A1	20040429	US 2003-659095	20030910

PRIORITY APPLN. INFO.: FR 2002-11213 A 20020911
OTHER SOURCE(S): MARPAT 140:253457
GI

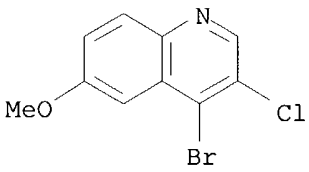
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1a = H, halo, OH, NH2, alkylamino, dialkylamino, hydroxyamino, alkoxyamino, or alkylalkoxyamino; R1b = H, or R1aR1b = oxo; R2 = COOH, CH2CO2H, CH2OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3 -7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = C1-6 alkyl, alkenyl-CH2, or alkynyl-CH2 (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including various isomers, enantiomeric and diastereoisomeric forms, mixts. and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Two synthetic examples are given. For example, II was prepd. by alkylation of III.bul.HCl (prepn. given) with

2-(bromoethylsulfanyl)thiophene, followed by basic hydrolysis. In vivo, compds. I were active against exptl. infections of mice by Staphylococcus aureus IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c.

IT **426842-71-9**, 4-Bromo-3-chloro-6-methoxyquinoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of quinolylpropyl piperidines as antimicrobial agents)

RN 426842-71-9 CA
CN Quinoline, 4-bromo-3-chloro-6-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 5 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 140:235614 CA
TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
INVENTOR(S): Bacque, Eric; Bigot, Antony; El Ahmad, Youssef; Malleron, Jean Luc; Mignani, Serge; Ronan, Baptiste; Tabart, Michel; Viviani, Fabrice
PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.
SOURCE: Fr. Demande, 66 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844270	A1	20040312	FR 2002-11212	20020911
WO 2004024712	A1	20040325	WO 2003-FR2686	20030910
W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, RO, SC, SG, SY, TN, TT, UA, UZ, VC, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004087619	A1	20040506	US 2003-659164	20030910

PRIORITY APPLN. INFO.: FR 2002-11212 A 20020911
OTHER SOURCE(S): MARPAT 140:235614
GI

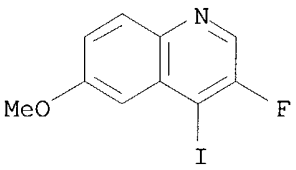
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H or F; R2 = COOH, CH2CO2H, CH2OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3 -7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = C1-6 alkyl, alkenyl-CH2, or alkynyl-CH2 (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including enantiomeric and diastereoisomeric forms, mixts. thereof, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Five synthetic examples are given. For example, II was prepd. by N-alkylation of III (prepn. given) with 2-[(2-bromoethyl)sulfanyl]-1,4-difluorobenzene, followed by acidic hydrolysis. Compds. I were active against exptl. infections of mice by Staphylococcus aureus IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT **426842-84-4**, 4-Iodo-3-fluoro-6-methoxyquinoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of quinolylpropylpiperidines as antimicrobials)

RN 426842-84-4 CA

CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 5 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 139:164798 CA
TITLE: Preparation of aminopiperidine derivatives for treatment of bacterial infections
INVENTOR(S): Miller, William Henry; Pearson, Neil David; Pendrak, Israil; Seefeld, Mark Andrew
PATENT ASSIGNEE(S): Glaxo Group Limited, UK; Daines, Robert A
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003064421	A1	20030807	WO 2003-EP823	20030127

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

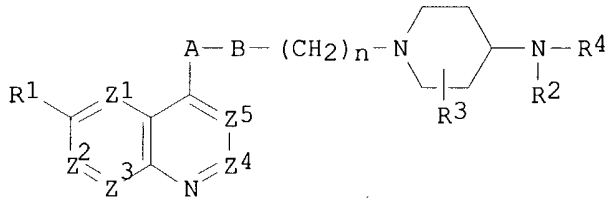
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: GB 2002-2026 A 20020129
GB 2002-29824 A 20021220

OTHER SOURCE(S): MARPAT 139:164798

GI



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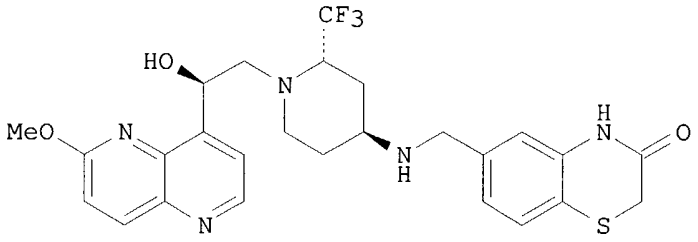
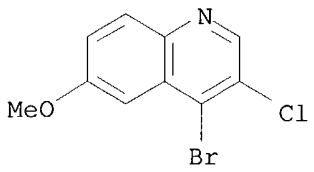


II

AB Title compds. I [one of Z1-5 = N, one = CR1a and the remainder = CH or one of Z1-5 = CR1a and the remainder = CH; R1-1a = H, OH, alkoxy, amino, etc.; R2 = H, alkyl, alkenyl; R3 = CF3, 2-oxo, etc.; R4 = UR5; U = CO, SO2, CH2; R5 = bicyclic, heterocyclic ring system A; n = 0-1; AB = amido, alkylacyl, aminosulfonyl, etc.] are prepd. For instance, bromomethyl (6-methoxy[1,5]naphthyridin-4-yl)ketone (prepn. given) is reduced (PhMe, (+)-DIPCl) to give the (R)-alc., converted to the oxirane (MeOH, K2CO3) and used to alkylate [(2S,4S)-2-(trifluoromethyl)piperidin-4-yl]carbamic acid tert-Bu ester (prepn. given) and deprotected to give (1R)-2-[(2S,4S)-4-amino-2-(trifluoromethyl)piperidin-1-yl]-1-(6-methoxy[1,5]naphthyridin-4-yl)ethanol. This amine is alkylated with 3-oxo-3,4-dihydro-2H-benzo[1,4]thiazine-6-carboxaldehyde (prepn. given) (EtOH, NaBH4) to give II. Selected examples have MICs .ltoreq. 2 .mu.g/mL vs., e.g., S. epidermidis CL7, S. aureus WCUH29, etc.

IT **426842-71-9P**, 4-Bromo-3-chloro-6-methoxyquinoline
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of aminopiperidine derivs. for treatment of bacterial

infections)
RN 426842-71-9 CA
CN Quinoline, 4-bromo-3-chloro-6-methoxy- (9CI) (CA INDEX NAME)



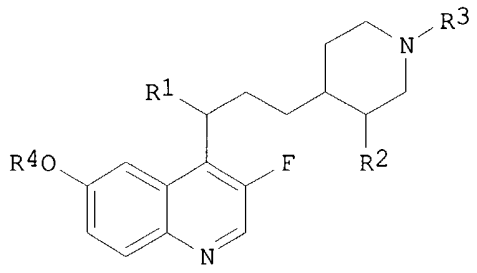
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 5 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 137:232568 CA
TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
INVENTOR(S): Bacque, Eric; Mignani, Serge; Malleron, Jean-Luc; Tabart, Michel; Evers, Michel; Viviani, Fabrice; El-Ahmad, Youssef; Mutti, Stephane; Daubie, Christophe
PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
SOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072572	A1	20020919	WO 2002-FR851	20020311
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2822154	A1	20020920	FR 2001-3374	20010313
EP 1370550	A1	20031217	EP 2002-722329	20020311
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2002177606	A1	20021128	US 2002-96482	20020313
US 6602884	B2	20030805		
US 2003171369	A1	20030911	US 2003-387479	20030314

PRIORITY APPLN. INFO.:
FR 2001-3374 A 20010313
US 2001-281407P P 20010405
WO 2002-FR851 W 20020311
US 2002-96482 A3 20020313

OTHER SOURCE(S): MARPAT 137:232568
GI



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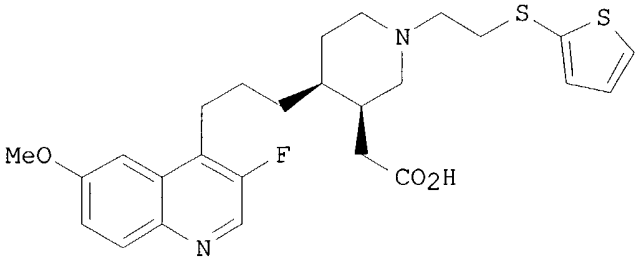


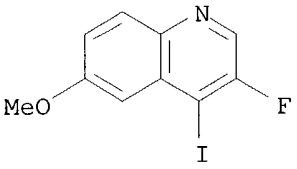
II

AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H, halo, OH, NH2, alkylamino, dialkylamino, hydroxyamino, alkoxyamino, or alkylalkoxyamino; R2 = COOH, CH2CO2H, CH2OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3 -7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = C1-6 alkyl, alkenyl-CH2, or alkynyl-CH2- (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including diastereoisomeric forms, mixts. thereof, cis or trans forms, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Ten synthetic examples are given. For instance, Wittig reaction of 4(RS)-4-allyl-1-(benzyloxycarbonyl)piperidin-3-one with Ph3P:CHCO2Me gave a Z-isomeric exocyclic olefin, which underwent hydroboration at allyl and Pd-catalyzed coupling with 4-iodo-3-fluoro-6-methoxyquinoline, followed by hydrogenation of the olefin with concomitant N-deprotection, N-alkylation with 2-(2-bromoethylthio)thiophene, and sapon. of the Me ester, to give the racemic title compd. II.2HCl. Compds. I were active against exptl. infections of mice by Staphylococcus aureus IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT **426842-84-4**, 4-Iodo-3-fluoro-6-methoxyquinoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(precursor; prepn. of (quinolylpropyl)piperidine derivs. as antimicrobials)

RN 426842-84-4 CA

CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 5 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 136:386033 CA
TITLE: Heterocyclylalkyl piperidine derivatives, particularly 4-[3-(quinolin-4-yl)propyl]piperidine-4-carboxylic acids, their preparation and compositions containing same, for use as antibacterials.
INVENTOR(S): Bacque, Eric; Carry, Jean-Christophe; El-Ahmad, Youssef; Evers, Michel; Hubert, Philippe; Malleron, Jean-Luc; Mignani, Serge; Pantel, Guy; Tabart, Michel; Viviani, Fabrice
PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
SOURCE: PCT Int. Appl., 362 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040474	A2	20020523	WO 2001-FR3559	20011114
WO 2002040474	A3	20021031		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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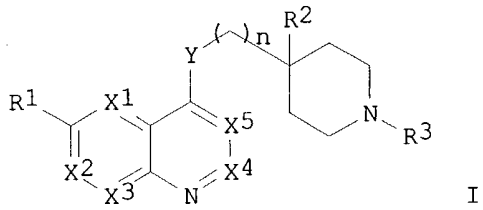
FR 2816618	A1	20020517	FR 2000-14738	20001115
FR 2816618	B1	20021227		
AU 2002018365	A5	20020527	AU 2002-18365	20011114
US 2002111492	A1	20020815	US 2001-987386	20011114
US 6603005	B2	20030805		
EE 200300207	A	20030815	EE 2003-207	20011114
EP 1337529	A2	20030827	EP 2001-996538	20011114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001015312	A	20030923	BR 2001-15312	20011114
JP 2004514661	T2	20040520	JP 2002-543484	20011114
NO 2003002187	A	20030626	NO 2003-2187	20030514

PRIORITY APPLN. INFO.:			
FR 2000-14738	A	20001115	
US 2000-255145P	P	20001214	
WO 2001-FR3559	W	20011114	

OTHER SOURCE(S): MARPAT 136:386033

GI



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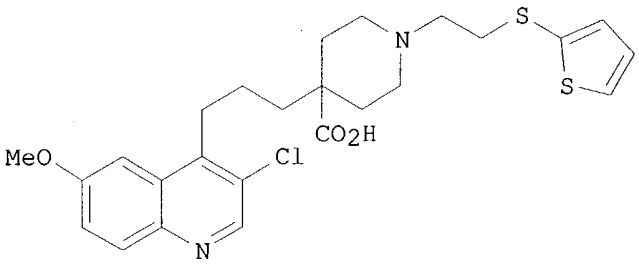


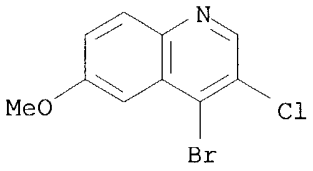
II

AB The invention concerns heterocyclylalkyl piperidine derivs. I, including their enantiomeric or diastereoisomeric forms, or mixts. thereof, and/or their syn or anti forms, or mixts. thereof, and their salts [wherein X1, X2, X3, X4, and X5 = C(R'1), C(R'2), C(R'3), C(R'4), C(R'5), or one of X-groups (at most) = N; R1, R'1, R'2, R'3, R'4, R'5 = H, halo, alkyl, cycloalkyl, Ph, PhS, OH, heterocyclyl, cyano, CO2H, alkoxycarbonyl, (un)substituted NH2, etc.; R2 = CO2H, alkyloxycarbonyl, cycloalkyloxycarbonyl, cyano, CONRaRb, CH2OH, substituted alkyl, CF2-Rc, C(CH3)2-Rc, CORc, CH(OH)-Rc, C(cycloalkyl)-Rc, or CH:CH-Rc; Ra, Rb = H, alkyl, cycloalkyl, Ph, heterocyclyl; or NRaRb = (un)substituted 5- or 6-membered heterocycle; Rc = CO2H, alkoxycarbonyl, cycloalkoxycarbonyl, CONRaRb; R3 = Ph, heterocyclyl, various substituted alkyls; Y = CH(Re), CF2, C(:NOH), alkyloxyiminomethylene, cycloalkyloxyiminomethylene, or C3-6 cycloalkylidene; Re = H, F, OH, alkoxy, cycloalkoxy, CO2H, alkoxycarbonyl, NRaRb, CONRaRb; and n = 0-4; wherein the radicals or Ph or heterocyclyl portions mentioned above can optionally be substituted]. Approx. 60 compds. were prepd., 5 were specifically claimed, and many more names were listed. For instance, Pd-complex-catalyzed coupling of 4-allyl-4-Cbz-1-BOC-piperidine with 4-bromo-3-chloro-6-methoxyquinoline (prepns. of both compds. given), followed by removal of the BOC group with CF3CO2H, N-alkylation with 2-[(2-bromoethyl)thio]thiophene, and hydrolysis of the benzyl ester (Cbz) in aq. HCl, gave title compd. II as the di-HCl salt. I are active against both gram-pos. and gram-neg. bacteria. I were active against exptl. infection of mice with Staphylococcus aureus IP8203 at 18-150 mg/kg s.c., or 20-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT **426842-71-9P**, 4-Bromo-3-chloro-6-methoxyquinoline
426842-84-4P, 4-Iodo-3-fluoro-6-methoxyquinoline
426842-86-6P, 4-Chloro-3-fluoro-6-methoxyquinoline
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of quinolinylpropylpiperidinecarboxylic acids as antibacterials.)

RN 426842-71-9 CA
CN Quinoline, 4-bromo-3-chloro-6-methoxy- (9CI) (CA INDEX NAME)



RN 426842-84-4 CA
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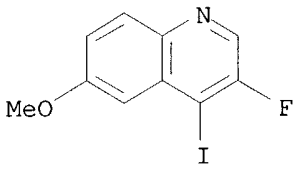

RN 426842-86-6 CA
CN Quinoline, 4-chloro-3-fluoro-6-methoxy- (9CI) (CA INDEX NAME)